# Numerical Mathematics
# Optimisation
# (Non-Examinable)

Pieter Collins

Department of Knowledge Engineering

Maastricht University

`pieter.collins@maastrichtuniversity.nl`

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# Optimisation Problems

## General Optimisation Problem

**Formalisation** Given a set $X$ and a function $f : X \to \mathbb{R}$, find $x^* \in X$ such that $f(x^*) \leq f(x)$ for all $x \in X$.

**Local Optimisation** Find a point $x^\dagger \in X$ such that for some $\epsilon > 0$, $f(x^\dagger) \leq f(x)$ whenever $d(x^\dagger, x) < \epsilon$.

## Continuous Optimisation

**Unconstrained** Feasible set $X$ is $\mathbb{R}^n$.

**One-Dimensional** Feasible set $X$ is an interval in $\mathbb{R}$.

## Optimality conditions (1d)

Let $f : [a, b] \to \mathbb{R}$ be sufficiently differentiable.

**Interior** $x$ is an interior point if $x \in (a, b)$.

**Necessary** If $f$ has an local minimum at $x$, then $f'(x) = 0$ and $f''(x) \geq 0$.

**Sufficient** If $f'(x) = 0$ and $f''(x) > 0$, then $x$ is a local minimum.

**Endpoints**

**Necessary** If $f$ has a local minimum at $a$, then $f'(a) \geq 0$.

**Sufficient** If $f'(a) > 0$, then $f$ has a local minimum at $a$.

## Optimality conditions

**Positive (semi)definite** A symmetric matrix $S$ is *positive-definite*, denoted $S \prec 0$, if $v^T S v > 0$ whenever $v \neq 0$.

**Necessary** If $f : \mathbb{R}^n \to \mathbb{R}$ has a local minimum at $x$, then $\nabla f(x) = 0$, and $\nabla^2 f(x)$ is positive semidefinite.

**Sufficient** If $\nabla f(x) = 0$, and $\nabla^2 f(x)$ is positive-definite, then $f : \mathbb{R}^n \to \mathbb{R}$ has a local minimum at $x$.

# Local Optimisation

## Unconstrained

**Quadratic approximation** Sufficient local information contained in *quadratic* terms.

**Line search** Compute $x_{k+1} = x_k + \alpha_k s_k$, where $s_k$ is a *search direction*, and $\alpha_k$ approximately minimises $f(x_k + \alpha s_k)$.

**Trust region** Approximate $f$ by $\tilde{f}$ in a sub-region $R$, and (approximately) minimise $\tilde{f}$ in $R$.

## Unconstrained Methods

**Hill climbing** Given a point $x$ and vectors $v_1, \ldots, v_m$, $m > n$, choose $v_i$ such that $f(x + v_i)$ is minimised, set $x_{n+1} = x_n + v_{n,i}$.

BAD. VERY, VERY BAD.

**Simplex** Given $n + 1$ points, choose new point outside simplex (search) or inside (refinement).

**Steepest-Descent** Choose search direction $s_k = -g_k$ where $g_k = \nabla f(x_k)$. BAD

**Conjugate-gradient** Choose search direction $s_k = -g_k + \beta_{k-1} s_{k-1}$ where $\beta_{k-1} = \frac{(g_k - g_{k-1})^T g_k}{g_{k-1}^T g_{k-1}}$.

**Newton** Choose search direction $s_k = -H_k^{-1} g_k$ where $H_k = \nabla^2 f(x_k)$.

Taking $\alpha_k = 1$, corresponds to minimising Taylor expansion $\tilde{f}_k(x) = f(x_k) + g_k(x - x_k) + \frac{1}{2} H_k (x - x_k)^2$.

**Quasi-Newton** Choose $s_k = -Q_k g_k$ where $Q_k \approx H_k^{-1}$ is computed using

# Global Optimisation

# Complexity

Global, non-convex problems may have many local minima.

Searching through these to find the best may take a lot of work.

Sharp, deep valleys are hard to find.

## Heuristics

**Random search** Aim to explore state space focusing on promising areas.

**Simulated annealing**

**Particle swarm**

**Genetic**

**Ant colony**

**Neural nets**

## Methods

**Branch-and-bound**

**Cutting**

**Lagrange relaxation**

## Future

**Morse Theory** Map out hills and saddles to find promising regions.